

# L-Proline, N-(5-chlorovaleryl)-, pentyl ester

**Inchi:** InChI=1S/C15H26ClNO3/c1-2-3-6-12-20-15(19)13-8-7-11-17(13)14(18)9-4-5-10-16/h13H  
**InchiKey:** UQYJFYSIAMOOPN-UHFFFAOYSA-N  
**Formula:** C15H26ClNO3  
**SMILES:** CCCCCOC(=O)C1CCCN1C(=O)CCCCCl  
**Mol. weight [g/mol]:** 303.82

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.47		Crippen Method
logp	3.120		Crippen Method
mcvol	242.580	ml/mol	McGowan Method
rinpol	2318.00		NIST Webbook
rinpol	2318.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346234&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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